



chain nodes :

1 2 3 4 5 6 7 14 15 16 23 24 33

ring nodes :

8 9 10 11 12 13 17 18 19 20 21 22 25 26 27 28 29 30

chain bonds :

1-2 2-3 3-4 3-5 5-6 6-7 7-9 12-14 14-15 14-16 16-17 20-23 23-24 24-27 30-33

ring bonds :

8-9 8-13 9-10 10-11 11-12 12-13 17-18 17-22 18-19 19-20 20-21 21-22 25-26 25-30
26-27 27-28 28-29 29-30

exact/norm bonds :

3-4 3-5 7-9 14-15 14-16 16-17 20-23 23-24 24-27 25-26 25-30 26-27 27-28 28-29
29-30

exact bonds :

1-2 2-3 5-6 6-7 12-14 30-33

normalized bonds :

8-9 8-13 9-10 10-11 11-12 12-13 17-18 17-22 18-19 19-20 20-21 21-22

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 33:CLASS